AD-A204 955

DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

Unclassified	1b. RESTRICTIVE MARKINGS: None
2a. SECURITY CLASSIFICATION AUTHORITY	3. DISTRIBUTION/AVAILABILITY OF REPORT: Approved for public release; distribution is unlimited
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE	
4. PERFORMING ORGANIZATION REPORT NUMBER(S): JA 330:042:82	5. MONITORING ORGANIZATION REPORT NUMBER(S): JA 330:042:82
6a. NAME OF PERFORMING ORGANIZATION: Naval Ocean Research and Development Activity; 6b. OFFICE SYMBOL (If applicable): 330	7a. NAME OF MONITORING ORGANIZATION: Ocean Science Directorate
6c. ADDRESS (City, State, and ZIP Code): Stennis Space Center, MS 39529-5004	7b. ADDRESS (City, State, and ZIP Code): Stennis Space Center, MS 39529-5004
8a. NAME OF FUNDING/SPONSORING ORGANIZATION: Naval Ocean Research and Development Activity; 8b. OFFICE SYMBOL (If applicable): 330	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER
8c. ADDRESS (City, State, and ZIP Code): Stennis Space Center, MS 39529-5004	10. SOURCE OF FUNDING NUMBERS: PROGRAM ELEMENT NO. 63704N; PROJECT NO.; TASK NO.; WORK UNIT ACCESSION NO. DN294462

11. TITLE (Include Security Classification)

A better least-squares method when both variables have uncertainties

12. PERSONAL AUTHOR(S)
Matthew Lybanon

13a. TYPE OF REPORT	13b. TIME COVERED	14. DATE OF REPORT (Year, Month, Day)	15. PAGE COUNT
Journal Article	FROM _____ TO _____	January 1984	5

16. SUPPLEMENTARY NOTATION

17. COSATI CODES			18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)
FIELD	GROUP	SUB-GROUP	Least squares, curve fitting, data analysis

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

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20. DISTRIBUTION/AVAILABILITY OF ABSTRACT	21. ABSTRACT SECURITY CLASSIFICATION	
☐ UNCLASSIFIED/UNLIMITED ☒ SAME AS RPT. ☐ DTIC USERS	Unclassified	
22a. NAME OF RESPONSIBLE INDIVIDUAL: Matthew Lybanon	22b. TELEPHONE (Include Area Code): 601-688-5263	22c. OFFICE SYMBOL: 332

DD Form 1473, JUN 86 *Previous editions are obsolete.* SECURITY CLASSIFICATION OF THIS PAGE: Unclassified

NAVAL OCEAN RESEARCH AND DEVELOPMENT ACTIVITY

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A better least-squares method when both variables have uncertainties

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reprint of an article in the American Journal of Physics
January 1984, Pages 22-26

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A better least-squares method when both variables have uncertainties

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(Received 27 December 1982; accepted for publication 29 April 1983)

The generalized least-squares problem, in which an observation vector satisfies a set of equations that may be nonlinear and implicit, and all components may be subject to errors, can be solved as a constrained minimization problem. When the analysis is specialized to the important case of one-dimensional curve fitting to measurements where both variables contain errors, it becomes similar to the effective variance method. A standard least-squares computer program can be used to apply the new method; the results are superior to those of the effective variance technique. A simple geometrical construction illustrates the principles of the new method.

I. INTRODUCTION

A recent paper by Jefferys[1] considered the generalized least-squares problem: A vector of observations satisfies a set of equations that may be nonlinear and is not necessarily solvable in the explicit form $y = f(x)$; all of the components of the vector of observations may be subject to measurement errors. The standard least-squares regression technique, even when extended to nonlinear models, contains the implicit assumption that x is free of error; this is hardly ever true in practice.

The method that Jefferys presents is more general than the conventional method and avoids the latter's inadequacies in formulation. Also, Jefferys makes two very important points:

(1) The standard method's assumption that one variable is subject to error and the other is error-free, when that assumption is inappropriate, produces biased estimates of the fit parameters. (Generalizations to higher dimensionality in all variables are included.) The bias is given explicitly by Jefferys for the case of a straight line through the origin where x, and not y, contains all the measurement uncertainty.

(2) The major difference between the standard least-squares solution procedure and the generalized method is that in the latter the expressions used in solving for the result must be recomputed each iteration using the best (i.e., revised) estimate of the observation vector as well as improved estimates of the fit parameters. This is a natural outgrowth of the notion that the least-squares process is a method of improving the observations via the mathematical model.[2] However, the point may not be obvious if one takes the common view of least squares solely as a method of parameter determination.

Other authors have treated the generalized least-squares problem; some have published iterative algorithms for fitting arbitrary functions to observation vectors all of whose components may possess uncertainty (as does Jefferys).[3-6] The principles have been discussed before in the American Journal of Physics.[7-11] Yet those principles and techniques seem not to be well-known. In particular, the results obtained by Jefferys[1] are remarkably similar to those of Britt and Luecke.[4] However, Jefferys appeared to be unaware of the existence of the Britt–Luecke paper, or indeed of any of the other works referred to by the present paper except (an earlier edition of) the book by Deming. (There is no intention to imply anything more than that the respective authors approached the problem in the same way. In fact, it is significant that Jefferys was apparently *not* aware of the other work, because that supports the contention that such methods are not well known.)

The work by Jefferys is highlighted here because the approach is general, and the formulation is concise and complete. In the next section the results presented by Jefferys will be summarized, using the same notation. Following that, it will be shown how the formalism, when applied to an important special case, results in an algorithm that has several advantages. That algorithm has pedagogical and practical value because it is particularly easy to use, gives better results than "effective-variance" techniques,[8] and has a convenient geometrical interpretation.

II. FORMULATION

A. General

Jefferys[1] formulated the least-squares problem as the minimization of a particular quadratic form,

$$S_0 = \tfrac{1}{2}\hat{\mathbf{v}}^t\boldsymbol{\sigma}^{-1}\hat{\mathbf{v}}, \tag{1}$$

subject to the constraints

$$\mathbf{f}(\mathbf{x}+\hat{\mathbf{v}},\hat{\mathbf{a}}) = \mathbf{0}, \tag{2}$$

$$\mathbf{g}(\hat{\mathbf{a}}) = \mathbf{0}. \tag{3}$$

In these equations x is a vector of observations with covariance matrix (assumed known at least up to a constant factor) $\boldsymbol{\sigma}$. The superscript "t" in Eq. (1) indicates transpose. Equation (2) is a set of *equations of condition*, in which $\mathbf{f}$ is a vector function of its arguments, $\mathbf{v}$ is the vector of actual residuals (i.e., $\mathbf{x} = \mathbf{x} + \mathbf{v}$ would have been the actual observations if there were no errors), and $\mathbf{a}$ is a vector of parameters. The same $\mathbf{v}$ appears in Eq. (1). Equation (3) is a set of constraints on the parameters $\mathbf{a}$. In all equations, a caret ($\hat{}$) above a symbol denotes an estimate of the quantity represented by that symbol.

A constrained minimization problem can be solved conveniently by the method of Lagrange multipliers, and that is the approach Jefferys chose. The statement of the problem becomes: Find estimates $\hat{\mathbf{v}}$ and $\hat{\mathbf{a}}$ of $\mathbf{v}$ and $\mathbf{a}$, and $\hat{\boldsymbol{\lambda}}$ and $\hat{\boldsymbol{\mu}}$ of the Lagrange multiplier vectors $\boldsymbol{\lambda}$ and $\boldsymbol{\mu}$, which minimize

$$S = \tfrac{1}{2}\hat{\mathbf{v}}^t\boldsymbol{\sigma}^{-1}\hat{\mathbf{v}} + \mathbf{f}^t(\hat{\mathbf{x}},\hat{\mathbf{a}})\hat{\boldsymbol{\mu}} + \mathbf{g}^t(\hat{\mathbf{a}})\hat{\boldsymbol{\lambda}}, \tag{4}$$

where $\mathbf{x} + \hat{\mathbf{v}}$ has been abbreviated by $\hat{\mathbf{x}}$. The minimization produces the *normal equations*

$$\boldsymbol{\sigma}^{-1}\hat{\mathbf{v}} + \mathbf{f}_x^t(\hat{\mathbf{x}},\hat{\mathbf{a}})\hat{\boldsymbol{\mu}} = \mathbf{0}, \tag{5a}$$

$$\mathbf{f}_a^t(\hat{\mathbf{x}},\hat{\mathbf{a}})\hat{\boldsymbol{\mu}} + \mathbf{g}_a^t(\hat{\mathbf{a}})\hat{\boldsymbol{\lambda}} = \mathbf{0}, \tag{5b}$$

$$\mathbf{f}(\hat{\mathbf{x}},\hat{\mathbf{a}}) = \mathbf{0} \tag{5c}$$

$$\mathbf{g}(\hat{\mathbf{a}}) = \mathbf{0}. \tag{15d}$$

In these equations the subscripts $\hat{\mathbf{x}}$,$\hat{\mathbf{a}}$ denote partial derivatives with respect to the indicated variables. The symbol $\mathbf{f}_{\mathbf{x}}$, for instance, is very compact notation for the matrix whose i,j element is $\partial f_i / \partial x_j$, evaluated at $\mathbf{x} = \hat{\mathbf{x}}$.

The solution to Eqs. (15a)–(15d) will give the solution to the posed problem, if it exists. However, these equations are in general nonlinear. The next step in Jefferys' approach is to apply Newton's method to linearize the equations about an approximate solution. Let the approximate solution be denoted by $(\hat{\mathbf{x}},\hat{\mathbf{a}})$, and let the linear estimate of the corrections be denoted by $(\hat{\boldsymbol{\epsilon}},\hat{\boldsymbol{\delta}})$. (The reader should note in particular that the solution includes all components of $\mathbf{x}$, as well as the parameters $\mathbf{a}$, and the distiction between $\hat{\boldsymbol{\epsilon}}$ and $\hat{\mathbf{v}}$ should be clear.) Then Eqs. (15a)–(15d) become

$$\boldsymbol{\sigma}^{-1}(\hat{\mathbf{v}} + \hat{\boldsymbol{\epsilon}}) + \mathbf{f}'_{\mathbf{x}}\hat{\boldsymbol{\mu}} = \mathbf{0}, \tag{16a}$$

$$\mathbf{f}'_{\mathbf{a}}\hat{\boldsymbol{\mu}} + \mathbf{g}'_{\mathbf{a}}\hat{\boldsymbol{\lambda}} = \mathbf{0}, \tag{16b}$$

$$\hat{\mathbf{f}} + \mathbf{f}_{\mathbf{x}}\hat{\boldsymbol{\epsilon}} + \mathbf{f}_{\mathbf{a}}\hat{\boldsymbol{\delta}} = \mathbf{0}, \tag{16c}$$

$$\hat{\mathbf{g}} + \mathbf{g}_{\mathbf{a}}\hat{\boldsymbol{\delta}} = \mathbf{0}. \tag{16d}$$

At this point, in anticipation of the special case to be discussed in the next section, the set of constraints on the parameters [Eq. (3)] will be dropped. This causes a slight simplification in the equations just stated; the second term in Eq. (16b) and all of Eq. (16d) vanish, and the Lagrange multipliers $\boldsymbol{\lambda}$ are no longer needed.

Continuing the solution, if Eq. (16a) is solved for $\hat{\boldsymbol{\epsilon}}$, the result is

$$\hat{\boldsymbol{\epsilon}} = -\hat{\mathbf{v}} - \boldsymbol{\sigma}\mathbf{f}'_{\mathbf{x}}\hat{\boldsymbol{\mu}}. \tag{17}$$

When this, in turn, is substituted into Eq. (16c),

$$\hat{\mathbf{f}} - \mathbf{f}_{\mathbf{x}}\hat{\mathbf{v}} - \mathbf{f}_{\mathbf{x}}\boldsymbol{\sigma}\mathbf{f}'_{\mathbf{x}}\hat{\boldsymbol{\mu}} + \mathbf{f}_{\mathbf{a}}\hat{\boldsymbol{\delta}} = \mathbf{0}, \tag{18}$$

which can be solved for the Lagrange multipliers

$$\hat{\boldsymbol{\mu}} = \mathbf{W}(\hat{\mathbf{f}} - \mathbf{f}_{\mathbf{x}}\hat{\mathbf{v}} + \mathbf{f}_{\mathbf{a}}\hat{\boldsymbol{\delta}}), \tag{19}$$

where the weighting matrix $\mathbf{W}$ is

$$\mathbf{W} = (\mathbf{f}_{\mathbf{x}}\boldsymbol{\sigma}\mathbf{f}'_{\mathbf{x}})^{-1}. \tag{20}$$

The (simplified) Eq. (16b) may now be solved to obtain the *reduced normal equation*

$$\mathbf{f}'_{\mathbf{a}}\mathbf{W}\mathbf{f}_{\mathbf{a}}\hat{\boldsymbol{\delta}} = -\mathbf{f}'_{\mathbf{a}}\mathbf{W}\hat{\boldsymbol{\phi}}, \tag{21}$$

where

$$\hat{\boldsymbol{\phi}} = \hat{\mathbf{f}} - \mathbf{f}_{\mathbf{x}}\hat{\mathbf{v}}. \tag{22}$$

The solution to Eq. (21) can be used to "update" the parameter estimates,

$$\hat{\mathbf{a}}_{\text{new}} = \hat{\mathbf{a}} + \hat{\boldsymbol{\delta}}. \tag{23}$$

But in order to complete the iterative process, it is also necessary to update $\mathbf{x}$,

$$\hat{\mathbf{x}}_{\text{new}} = \hat{\mathbf{x}} + \hat{\boldsymbol{\epsilon}}. \tag{24}$$

Equation (16a) may be used to find $\hat{\boldsymbol{\epsilon}}$. After substituting $\hat{\boldsymbol{\mu}}$ from Eq. (19) and performing some manipulations, the final result is

$$\hat{\mathbf{x}}_{\text{new}} = \mathbf{x} + \hat{\mathbf{v}}_{\text{new}}, \tag{25}$$

where

$$\hat{\mathbf{v}}_{\text{new}} = -\boldsymbol{\sigma}\mathbf{f}'_{\mathbf{x}}\mathbf{W}(\hat{\boldsymbol{\phi}} + \mathbf{f}_{\mathbf{a}}\hat{\boldsymbol{\delta}}). \tag{26}$$

This is equivalent to Eq. (23).

Jefferys suggests using $\hat{\mathbf{x}} = \mathbf{x}$ as an initial estimate of $\mathbf{x}$ (again, it must be emphasized that $\mathbf{x}$ will change), along with some vector $\mathbf{a}$ of initial parameter "guesses" for $\hat{\mathbf{a}}$. The solution process consists of solving Eq. (21) for $\hat{\boldsymbol{\delta}}$, using the current estimates of everything, then substituting the resulting $\hat{\boldsymbol{\delta}}$ into Eq. (26) to obtain $\hat{\mathbf{v}}_{\text{new}}$. Equations (23) and (25) then give improved values of $\hat{\mathbf{a}}$ and $\hat{\mathbf{x}}$. This constitutes one iteration. Successive iterations are performed, if necessary, until a set of convergence criteria are met, or until a prespecified large number of iterations are performed without reaching convergence. The latter method of stopping the calculation may be necessary for one of two reasons: If the problem is sufficiently complex and the initial estimates are too far away, this linearized algorithm may not converge to the solution at all. Or even if it does converge, the finite (limited) precision of the machine may not permit satisfaction of a severe convergence test.

The reason for duplicating Jefferys' formulation here in such detail is so that we can go from the general to the specific in the next section with a minimum of effort but with confidence in the validity of the results. The resulting algorithm will be amenable to a particularly simple implementation.

B. One-dimensional curve fitting

The preceding section has been entirely general. It treated the least-squares fitting of any relationship of the form $\mathbf{f}(\mathbf{x}) = \mathbf{0}$, where $\mathbf{x}$ is a vector of observations (and the dependence on the adjustable parameters has been suppressed). By far the most frequent application of least squares is to cases in which the functional relationship has the explicit form

$$y = u(x), \tag{27}$$

where both x and y are scalars. There is some slight confusion in notation; the components of $\mathbf{x}$ for the ith observation are $(x_i,y_i)(i = 1,2,\ldots,N$, where N, is the number of observations). The vector function $\mathbf{f}(\mathbf{x})$ has N components, $f_i = u(x_i,\mathbf{a}) - y_i$. The vector of parameters $\mathbf{a}$ has m components. We assume uncorrelated measurements (x_i,y_i), so the matrix $\boldsymbol{\sigma}$ is diagonal.

A few of the matrices will be displayed explicitly, along with their dimensions:

$$\boldsymbol{\sigma} = \begin{bmatrix} \sigma_{x1}^2 & 0 & 0 & \cdots & 0 \\ 0 & \sigma_{y1}^2 & 0 & \cdots & 0 \\ 0 & 0 & \sigma_{x2}^2 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ 0 & 0 & 0 & \cdots & \sigma_{yN}^2 \end{bmatrix} \quad (2N \times 2N), \tag{28}$$

$$\mathbf{f}_{\mathbf{x}} = \begin{bmatrix} \dfrac{\partial u_1}{\partial x_1} & -1 & 0 & 0 & \cdots & 0 \\ 0 & 0 & \dfrac{\partial u_2}{\partial x_2} & -1 & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & -1 \end{bmatrix} \quad (N \times 2N), \tag{29}$$

$$\mathbf{f}_{\hat{\mathbf{a}}} = \begin{bmatrix} \frac{\partial u_1}{\partial a_1} & \frac{\partial u_1}{\partial a_2} & \cdots & \frac{\partial u_1}{\partial a_m} \\ \frac{\partial u_2}{\partial a_1} & \frac{\partial u_2}{\partial a_2} & \cdots & \frac{\partial u_2}{\partial a_m} \\ \vdots & \vdots & & \vdots \\ \frac{\partial u_N}{\partial a_1} & \frac{\partial u_N}{\partial a_2} & \cdots & \frac{\partial u_N}{\partial a_m} \end{bmatrix} \quad (N \times m). \tag{20}$$

The partial derivatives in Eqs. (19) and (20) are evaluated at $(\hat{x},\hat{\mathbf{a}})$ at each stage of the iterative calculation. The vector of actual residuals is

$$\hat{\mathbf{v}} = \begin{bmatrix} \hat{x}_1 - x_1 \\ \hat{y}_1 - y_1 \\ \hat{x}_2 - x_2 \\ \vdots \\ \hat{y}_N - y_N \end{bmatrix} \quad (2N \times 1). \tag{21}$$

In Eq. (21), $\hat{y}_i = \hat{u}(x_i)$.

Using these relations, it can be seen that $\mathbf{f}_x \boldsymbol{\sigma} \mathbf{f}_x'$ is now an $N \times N$ diagonal matrix whose ith diagonal element is $(\partial u_i / \partial x_i)^2 \sigma_{x_i}^2 + \sigma_{y_i}^2$. Consequently, Eq. (10) shows that the weighting matrix $\mathbf{W}$ is also an $N \times N$ diagonal matrix, whose ith diagonal element is

$$W_i = \left[\left(\frac{\partial u_i}{\partial x_i} \right)^2 \sigma_{x_i}^2 + \sigma_{y_i}^2 \right]^{-1}. \tag{22}$$

And the vector $\hat{\boldsymbol{\phi}}$, defined in Eq. (12), is the $N \times 1$ vector whose ith element is

$$\hat{\phi}_i = -\left(y_i - u(\hat{x}_i,\hat{\mathbf{a}}) - \frac{\partial u}{\partial x_i}(x_i - \hat{x}_i) \right). \tag{23}$$

[Once again, the partial derivatives in both equations are evaluated at $(\hat{x},\hat{\mathbf{a}})$.]

Reference to Fig. 1 (which suppresses the index i) shows that $\hat{\phi}_i$ is the negative of the quantity shown as d (i.e., d_i):

$$\hat{\phi}_i = -d_i. \tag{24}$$

Note furthermore that, to a good approximation,

$$\hat{\phi}_i \simeq -R_i = u(x_i,\hat{\mathbf{a}}) - y_i. \tag{25}$$

Figure 1 depicts the region near one observation in a space with (x,y) normalized so that the variances at that point are unity. From Eqs. (1) and (21) it can be seen that the sum of squares S_0 reduces to a sum of terms of the form $\frac{1}{2}D_i^2$, where the line of length D_i is a perpendicular from (x,y) to the curve at $(\hat{x},u(\hat{x}))$. This provides a convenient geometrical interpretation of generalized least squares for this important special case.

It is now possible to carry out Jefferys' solution procedure. The first step is to solve Eq. (11) for $\hat{\boldsymbol{\delta}}$. In the present case,

$$(\mathbf{f}_{\mathbf{a}}' \mathbf{W} \mathbf{f}_{\mathbf{a}})_{ij} = \sum_{k=1}^{N} \frac{\partial u_k}{\partial a_i} W_k \frac{\partial u_k}{\partial a_j}, \tag{26a}$$

$$(\mathbf{f}_{\mathbf{a}}' \mathbf{W} \boldsymbol{\phi})_j = -\sum_{n=1}^{N} \frac{\partial u_n}{\partial a_j} W_n d_n \simeq -\sum_{n=1}^{N} \frac{\partial u_n}{\partial a_j} W_n R_n. \tag{26b}$$

Consequently, with the second form of Eq. (26b), Eq. (11) is exactly the equation obtained for the successive differential corrections to the parameters in the standard least-squares method, with two exceptions:

(1) All of the partial derivatives, with respect to both x and $\mathbf{a}$, are evaluated at $(\hat{x},\hat{\mathbf{a}})$ instead of $(x,\hat{\mathbf{a}})$.

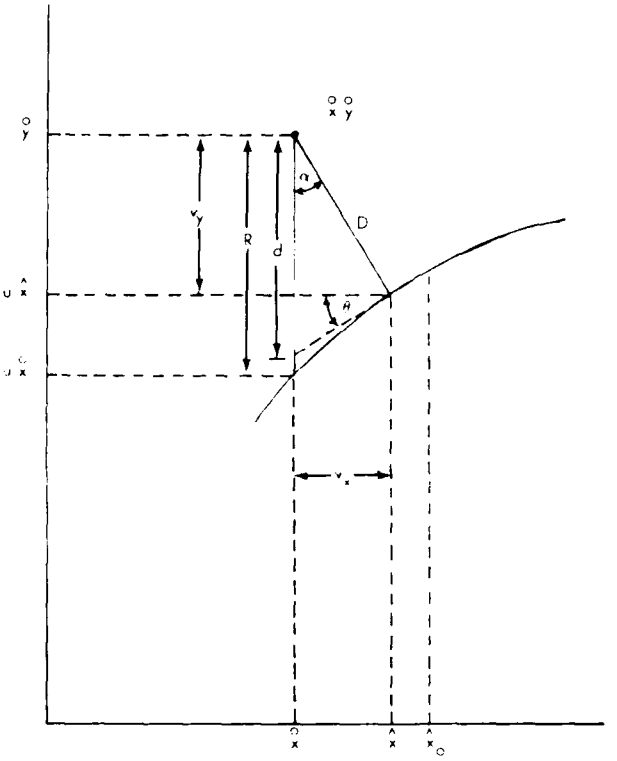

Fig. 1. Least-squares geometry in transformed space with unit variances.

(2) The weights in the W matrix are of the form

$$W_i = \left[\left(\frac{\partial u_i}{\partial x_i} \right)^2 \sigma_{x_i}^2 + \sigma_{y_i}^2 \right]^{-1}. \tag{27}$$

These are the effective variance weights.[8] They have been shown previously to be the appropriate weights to use for least squares when both x and y observations are subject to error.[14,15] However, the effective-variance *algorithm* described in those references neglected the other "exception" above. Consequently, it has been found that it almost never gives an exact least-squares solution.[16]

Because the method derived in this section is formally identical to standard least squares, with the exceptions noted above, it has the very important practical advantage that it can be implemented simply by making slight modification to existing curve fit computer software. The standard method effectively assumes that there are no x residuals—in other words, that there is no uncertainty in the x observations. Consequently, it is not applicable when there are x uncertainties. When it is applied in such cases it produces biased fits, as Jefferys showed.[1] However, with the relatively minor changes indicated above, a computer program that was designed for the standard method can be used for the general problem.

The approximation of replacing d_i by R_i still remains, so it may appear that the result of all the foregoing algebra was just to replace one approximate method—effective variance—with another. But it will be seen that the new method is a much better approximation than the effective variance technique, while retaining the latter's ease of implementation. Further, Fig. 1 provides a consistent geometrical interpretation of the method that is of pedagogical value. The use of the Figure will continue below.

The one missing element is a method of improving the x

estimates, in order that we may evaluate the partial derivatives at $\hat{x}$ rather that x. From Eqs. (7) and (14)–(16),

$$\hat{\boldsymbol{\epsilon}} = -\mathbf{v} - \boldsymbol{\sigma}\mathbf{f}_x'\hat{\boldsymbol{\mu}} = \mathbf{x} - \hat{\mathbf{x}} - \boldsymbol{\sigma}\mathbf{f}_x'\mathbf{W}(\hat{\boldsymbol{\phi}} + \mathbf{f}_a\hat{\boldsymbol{\delta}}). \tag{28}$$

Equation (28) is for the general case. If we now specialize to one-dimensional curve fitting and drop the $\mathbf{f}_a\hat{\boldsymbol{\delta}}$ term, which is a first-order correction to the "updated" $\hat{\mathbf{a}}$ (i.e., $\hat{\mathbf{a}} + \hat{\boldsymbol{\delta}}$), then the correction to $\hat{x}_i$ is

$$\begin{aligned}\delta\hat{x}_i &= x_i - \hat{x}_i - \sigma_{x_i}^2\frac{\partial u_i}{\partial x_i}W_i\hat{\phi}_i \\ &= x_i - \hat{x}_i - \sigma_{x_i}^2 \\ &\quad\cdot\frac{\partial u_i}{\partial x_i}\left(\hat{u}_i - y_i + \frac{\partial u_i}{\partial x_i}(x_i - \hat{x}_i)\right) \\ &\quad\cdot\left[\left(\frac{\partial u_i}{\partial x_i}\right)^2\sigma_{x_i}^2 + \sigma_{y_i}^2\right]^{-1},\end{aligned} \tag{29}$$

where $\hat{u}_i$ stands for $u(\hat{x}_i, \hat{\mathbf{a}})$. If we now define the separate x and y weights

$$W_{x_i} = 1/\sigma_{x_i}^2,\ W_{y_i} = 1/\sigma_{y_i}^2, \tag{30}$$

then Eq. (29) becomes

$$\begin{aligned}\delta\hat{x}_i &= \left(W_{x_i}(y_i - \hat{u}_i)\frac{\partial u_i}{\partial x_i} + W_{x_i}(x_i - \hat{x}_i)\right) \\ &\quad\cdot\left[W_{x_i}\left(\frac{\partial u_i}{\partial x_i}\right)^2 + W_{y_i}\right]^{-1}.\end{aligned} \tag{31}$$

Figure 1 provides an immediate geometrical interpretation. Assume that $\sigma_x = \sigma_y = 1$. (Again, we suppress the index i.) Then the line of length D is perpendicular to the curve and has the equation

$$y(x) - y = -\left(\frac{\partial u}{\partial x}\right)^{-1}(x - x). \tag{32}$$

Now suppose that we have an $\hat{x}_0$ that is an approximation and wish to find a better one, $\hat{x}$. The curve near $\hat{x}_0$ is given by, to first order,

$$u(x,\hat{\mathbf{a}}) = u(\hat{x}_0,\hat{\mathbf{a}}) + \frac{\partial u}{\partial x}\delta\hat{x}, \tag{33}$$

where $\delta\hat{x} = x - \hat{x}_0$. The needed correction from $\hat{x}_0$ to x is given by the simultaneous solution of Eqs. (32) and (33). The result is

$$\delta\hat{x} = \left((y - \hat{u})\frac{\partial u}{\partial x} + x - \hat{x}_0\right)\Big/\left[\left(\frac{\partial u}{\partial x}\right)^2 + 1\right]. \tag{34}$$

When the variables are "unnormalized" (transformed to arbitrary variances) and allowance is made for the slight changes in notation, Eq. (34) becomes identical to Eq. (31).

Following Jefferys' suggested algorithm of the preceding section, a sketch of the solution procedure for one-dimensional curve fitting when x and y contain measurement error is as follows: Eq. (31) gives the updates to the independent variable. With the weights (22), Eqs. (26a) and (26b) give the factors which go into Eq. (11) for the parameter updates. In this case Eq. (11) is exactly that used to give parameter updates in standard least squares, except that the partial derivatives are evaluated at the improved $\hat{x}_i$ and the special choice of weights (22) is used. Equation (11) is iterated until a convergence test is passed or an iteration limit is reached. The updates will change the weights, so the entire procedure (variable updates and parameter updates) is iterated until a suitable convergence criterion, such as the effective variance criterion proposed by Clutton-Brock,[14] is satisified. It may also be desirable to check the convergence of the independent variable estimates. The overall sum of squares of residuals is another candidate for a convergence check, since that is what is supposed to be minimized.

Table I. Pearson's data and York's weights.

i	x_i	W_{x_i}	y_i	W_{y_i}
1	0.0	1000.0	5.9	1.0
2	0.9	1000.0	5.4	1.8
3	1.8	500.0	4.4	4.0
4	2.6	800.0	4.6	8.0
5	3.3	200.0	3.5	20.0
6	4.4	80.0	3.7	20.0
7	5.2	60.0	2.8	70.0
8	6.1	20.0	2.8	70.0
9	6.5	1.8	2.4	100.0
10	7.4	1.0	1.5	500.0

III. EXAMPLES AND COMPARISON OF METHODS

The method described in the last section was programmed and applied to several cases. The same program ("built" around a standard least-squares program) was used to perform least squares and effective variance fits. The results are summarized below, along with published[5] exact generalized least-squares results.

The cases consisted of polynomial fits to data given by Pearson, who analyzed the problem of performing linear fits to measurements with error in all variables as long ago as 1901.[17] The weights [cf. Eq. (30)] used consisted of two sets: unit weights on both x and y, all points, and a set of weights used with Pearson's data by York.[18] Pearson's data and York's weights are listed in Table I.

Table II shows the results of fits of a straight line, $y = a_1 + a_2x$, to the data of Table I. S was calculated from

$$S = \sum_{i=1}^{N}\left[W_{x_i}(\hat{x}_i - x_i)^2 + W_{y_i}(\hat{y}_i - y_i)^2\right], \tag{35}$$

Table II. Linear fits to Pearson's data with York's weights.

Calculated value	Standard least squares	Effective variance	New algorithm	Exact solution
a_1	6.10010945	5.39605212	5.47991025	5.47991022
a_2	0.610812967	0.463448885	0.480533415	0.480533407
S	16.285266046	11.95644908	11.8663531941	11.8663531941

Table III. Polynomial fits to Pearson's data with unit weights or York's weights.

Polynomial degree	Weights	S for: Standard least squares	Effective variance	New algorithm	Exact solution
1	Unit	0.620119636654	0.620119636554	0.618572759437	0.618572759437
1	York	16.285266046	11.95644908	11.8663531941	11.8663531941
3	Unit	0.487316948683	0.486175535205	0.485155481449	0.485152486927
3	York	11.8832634403	10.5919459561	10.4878374498	10.4869040577
5	Unit	0.453000717248	0.453000307869	0.450329966231	0.450325667217

which is equivalent to Eq. (1) except for the factor of 1/2. The values $\hat{x}_i$ are calculated directly as a by-product of the calculation for the fits by the new algorithm and the exact solution. For the other fits, Eq. (31) was used to find the $\hat{x}_i$ consistent with the fit parameters, in order to be able to calculate S. The results show that the standard least-squares solution is seriously in error and the effective variance solution is substantially better, but the result of the new algorithm is identical to the exact solution within the precision of the calculation. The latter happens because no approximation is made by the new algorithm for linear fits, since d_i is exactly the same as R_i. The effective variance algorithm is not exact; since $\partial u_i/\partial a_2 = x_i$, the failure to update x_i in the effective variance calculation prevents the normal equation from producing a true minimum even though the weights are formally correct.

Table III shows the values of S obtained using each of the fit procedures for various polynomial fits to Pearson's data with either unit weights or York's weights. An interesting situation occurs in the case of straight-line fits with unit weights. The value of S for the effective variance fit is the same as that for the standard least-squares fit. The two fits are actually the same; the sets of coefficients are identical, also. This result is not unexpected. Chandler[16] showed that, for straight-line fits with $\sigma_{x_i} = \sigma$ and $\sigma_{y_i} = \tau$ for all i, the effective variance algorithm gives the same result as standard least squares. That solution is seen to be less than optimum, but the result of the new algorithm is again identical to the exact solution.

For polyomial fits of higher degree, the new algorithm is not exact. It is very nearly so, however, and it outperforms the effective variance algorithm in every case. On a linear scale which measures the percentage decrease in S from the standard least-squares result to the exact solution, the effective variance method attained an average "score" of 48.638%, while the new algorithm averaged 99.927%.

The relative differences between coefficient values for the different methods were even greater than the corresponding differences between S values. In particular, in the quintic polynomial fits the standard least squares and effective variance algorithms yielded some coefficients with sign differences compared to the exact solution, while the new algorithm's result agreed very closely. The new algorithm has also been used successfully to fit functions that depend nonlinearly on the fit parameters. However, the cases presented are widely used in the literature as standard test cases, permitting easy comparison with other methods.

IV. CONCLUSION

The standard least-squares procedure should not be used to perform curve fits when both x and y contain measurement uncertainty, because the underlying assumptions are violated and the method produces biased estimates of the fit parameters.[1] The effective variance technique, which has been recommended in this Journal for use in such cases,[8,15] is usually better but is still not exact. A new method, which can be obtained as the result of specializing an analysis of the generalized least-squares problem[1] to the case of one-dimensional curve fits to uncorrelated observations, gives better results but is no harder to use. One slight approximation makes the new method formally identical to the effective variance approach with one enhancement, so it shares the latter method's advantage that it can be applied using a standard least squares computer program. Tests prove that the new method is exact for linear regression (while the effective variance method is no better than standard least squares when all the x uncertainties are equal and all the y uncertainties are equal) and performs better than the effective variance method in other cases. There is a convenient geometrical interpretation; in a sense the new method is completely described by Fig. 1.

The new method is genuinely easy to apply using a standard least-squares algorithm. A microcomputer implementation can be used to fit arbitrary functions. The author has programmed the method for straight lines on the Texas Instruments TI-59 programmable pocket calculator, using the calculator's built-in straight-line-fit capability. That program is available on request.

The method introduced in the paper is an outgrowth of procedures developed for calibration of the measurements made in Skylab Experiment S-233, photographic photometry of Comet Kohoutek observations.

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